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FUNCTIONALS FOR FLUX SYNTHESIS WITH DISCONTINUOUS TRIAL FUNCTIONS

by

P. Lambropoulos and
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Reactor Physics Division

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ERRATUM

Page 5, paragraph two under "INTRODUCTION," please change line 3 to read:

...divergences, it has been deemed necessary to...

Alvin Glassner

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Technical Publications Department

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ABSTRACT

It is shown that the functionals originally used in variational flux synthesis with continuous trial functions can also be used with discontinuous functions, provided they are modified so as to yield physically meaningful stationarity conditions at the discontinuity interfaces. It is furthermore demonstrated that various functionals proposed in the past for such use are equivalent, without any among them having any added validity. Some mathematical difficulties that had been attributed to the use of discontinuous trial functions are clarified and shown to have been the result of inappropriate calculational methods.

INTRODUCTION

The functionals originally used[1] to formulate the methods of variational flux synthesis had the second-order diffusion equation and its adjoint as their Euler-Lagrange necessary conditions for stationarity. The class of admissible or trial functions used was the class of functions that are continuous in the reactor volume, with sectionally (or piecewise) continuous first derivatives.

It has often been stated[2,3] that such functionals will not remain finite when the class of admissible functions includes sectionally continuous functions. To avoid these divergences, we have deemed it necessary to introduce special functionals[2] having first-order Euler-Lagrange equations. It has also been stated[2,3] that the value of this new type of functional is ambiguously defined when evaluated with discontinuous trial functions.

This report shows that the aforementioned divergences and ambiguities do not arise if the trial functions are consistently interpreted as sectionally continuous functions, with sectionally continuous first derivatives. Then it will be seen that, to obtain physically meaningful stationarity conditions at the discontinuity interfaces, one needs to modify both the first- and the second-order functionals. However, the various modified functionals that will generate the appropriate interface conditions are not uniquely determined. They are all equivalent without any among them having any added validity.

The following section is devoted to the derivation and discussion of the various functionals for discontinuous trial functions. The list of such functionals presented in this report should be considered as representative rather than as exhaustive.

The last section takes up some pertinent mathematical problems. It is shown there that the apparent divergences and ambiguities have been caused by the use of inappropriate calculational methods and not by the discontinuous trial functions.

EVALUATION OF THE FUNCTIONALS

The functionals originally used to formulate the method of variational flux synthesis with continuous trial functions are of the type

$$J[\varphi,\varphi^*] = \int_a^b \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi\right) dx. \tag{1}$$

The type proposed to be used with discontinuous trial functions is

$$F[\varphi,\varphi^*,j,j^*] = \int_a^b \left(\varphi^* \frac{dj}{dx} - j^* \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi - j^* D^{-1} j\right) dx. \tag{2}$$

For simplicity, a one-dimensional system extending from $x = a$ to $x = b$ has been assumed, and all the nondiffusion terms in the group-diffusion operator have been lumped together into the Λ operator. For the same reason, the time dimension has been excluded and zero flux and adjoint boundary conditions will be imposed throughout. Any or all of these limitations could be removed without affecting the argument.

The classes of admissible functions to be used in the evaluation of the functionals are: for $J[\varphi,\varphi^*]$, the class of functions $\varphi(x)$ and $\varphi^*(x)$ that are sectionally continuous[4] with sectionally continuous first derivatives in $[a,b]$, assuming zero values at $x = a$ and $x = b$; for $F[\varphi,\varphi^*,j,j^*]$, the same class of functions $\varphi(x)$ and $\varphi^*(x)$, plus the class of functions $j(x)$ and $j^*(x)$ that are sectionally continuous with sectionally continuous first derivatives in $[a,b]$.

The term "sectionally continuous" is used here in the conventional sense, and it implies that the function in question is continuous almost everywhere in $[a,b]$, that is, at all points except for a set of points of measure zero. For the purposes of this report, such a set will be assumed to consist of a finite number of points. At the points of discontinuity, the value of the function is assumed to have finite (but different) limits from the left and the right. This type of discontinuity will be referred to as jump discontinuity. (These conditions could be relaxed to admit discontinuous functions with unbounded limits from either side, provided such functions were square integrable.)

Again for the sake of simplicity, we will assume that there is only one point ($x = x_0$) inside $[a,b]$ where the functions φ, φ^*, $d\varphi/dx$, $d\varphi^*/dx$, j, and j^* can have a jump discontinuity. At that point x_0, the derivatives $d\varphi/dx$, $d\varphi^*/dx$, dj/dx, and dj^*/dx do not exist. The functions φ and φ^* may or may not be defined at $x = x_0$.

The functionals $J[\varphi,\varphi^*]$ and $F[\varphi,\varphi^*,j,j^*]$, being the integrals of sectionally continuous functions, are now well defined, finite, and given by[5]

$$J[\varphi,\varphi^*] = \int_a^b \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi\right) dx$$

$$= \int_a^{x_0^-} \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi\right) dx + \int_{x_0^+}^b \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi\right) dx, \tag{3}$$

and

$$F[\varphi,\varphi^*,j,j^*] = \int_a^b \left(\varphi^* \frac{dj}{dx} - j^* \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi - j^* D^{-1} j\right) dx$$

$$= \int_a^{x_0^-} \left(\varphi^* \frac{dj}{dx} - j^* \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi - j^* D^{-1} j\right) dx$$

$$+ \int_{x_0^+}^b \left(\varphi^* \frac{dj}{dx} - j^* \frac{d\varphi}{dx} + \varphi^* \Lambda \varphi - j^* D^{-1} j\right) dx. \tag{4}$$

The integral

$$\int_a^{x_0^-} f(x)\, dx + \int_{x_0^+}^b f(x)\, dx$$

is a short-hand notation for

$$\lim_{\varepsilon \to +0}\left(\int_a^{x_0-\varepsilon} f(x)\,dx + \int_{x_0+\varepsilon}^{b} f(x)\,dx\right),$$

where the limit is taken after the integration is performed. It is in this sense that all integrals over [a,b] should be understood in this report. For the class of functions considered here, such integrals will always be finite and independent of whatever value one might assign to the function at x_0, for this is a set of measure zero. Moreover, since the functions in question are continuous in each of the intervals $[a, x_0 - \varepsilon]$ and $[x_0 + \varepsilon, b]$, one can integrate by parts and then take the limit for $\varepsilon \to +0$. Using this procedure of integration by parts in Eq. 3, one finds that the functional $J[\varphi,\varphi^*]$ can be written in two other equivalent forms; i.e.,

$$J[\varphi,\varphi^*] = \varphi_-^* D_- \varphi_-' - \varphi_+^* D_+ \varphi_+' + \int_a^b \varphi^* \left[-\frac{d}{dx}\left(D\,\frac{d\varphi}{dx}\right) + \Lambda\varphi\right] dx, \tag{5}$$

or

$$J[\varphi,\varphi^*] = \varphi_-^{*\prime} D_- \varphi_- - \varphi_+^{*\prime} D_+ \varphi_+ + \int_a^b \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}\,D\right) + \varphi^*\Lambda\right] \varphi\,dx, \tag{6}$$

where

$$\lim_{\varepsilon\to 0} D(x_0 - \varepsilon) = D_-,$$

$$\lim_{\varepsilon\to 0} D(x_0 + \varepsilon) = D_+,$$

$$\lim_{\varepsilon\to 0} \varphi(x_0 - \varepsilon) = \varphi_-,$$

$$\lim_{\varepsilon\to 0} \varphi(x_0 + \varepsilon) = \varphi_+,$$

$$\lim_{\varepsilon\to 0} \left.\frac{d\varphi}{dx}\right|_{x_0-\varepsilon} = \varphi_-',$$

and

$$\lim_{\varepsilon\to 0} \left.\frac{d\varphi}{dx}\right|_{x_0+\varepsilon} = \varphi_+',$$

and similarly for φ^* and its derivatives. Note that if a function has a jump discontinuity, say at x_0, its derivative may approach infinity from the left and/or the right. One can readily show, however, that this will be an integrable singularity. Therefore, since, for example, $d\varphi(x)/dx$ is assumed to have only jump discontinuities, the integral

$$\int_a^b \varphi^* \frac{d}{dx} D \frac{d\varphi}{dx}\, dx$$

will be finite (provided of course, that $D(x)$ is bounded and differentiable, which is assumed to be the case).

By means of the same transformation, the functional F can be written in three other equivalent forms:

$$F[\varphi,\varphi^*,j,j^*] = \varphi^*_- j_- - \varphi^*_+ j_+ + \int_a^b \left(- \frac{d\varphi^*}{dx} j - j^* \frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \qquad (7)$$

or

$$F[\varphi,\varphi^*j,j^*] = j^*_+\varphi_+ - j^*_-\varphi_- + \int_a^b \left(\varphi^* \frac{dj}{dx} + \frac{dj^*}{dx} \varphi + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \qquad (8)$$

or

$$F[\varphi,\varphi^*j,j^*] = \varphi^*_- j_- - \varphi^*_+ j_+ - j^*_-\varphi_- + j^*_+\varphi_+ + \int_a^b \left(\frac{dj^*}{dx} \varphi - \frac{d\varphi^*}{dx} j\right.$$

$$\left. + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \qquad (9)$$

where, as before j_-, j_+, j^*_-, and j^*_+ indicate limiting values of these functions at $x = x_0$.

The stationarity conditions for $J[\varphi,\varphi^*]$ and $F[\varphi,\varphi^*j,j^*]$ can be obtained from any of their equivalent forms. Using Eqs. 1 and 2 results in

$$\delta J = \int_a^b \left(\frac{d\delta\varphi^*}{dx} D \frac{d\varphi}{dx} + \frac{d\varphi^*}{dx} D \frac{d\delta\varphi}{dx} + \delta\varphi^*\Lambda\varphi + \varphi^*\Lambda\delta\varphi\right) dx, \qquad (10a)$$

and

$$\delta F = \int_a^b \left(\delta\varphi^* \frac{dj}{dx} + \varphi^* \frac{d\delta j}{dx} - \delta j^* \frac{d\varphi}{dx} - j^* \frac{d\delta\varphi}{dx} + \delta\varphi^*\Lambda\varphi + \varphi^*\Lambda\delta\varphi\right.$$

$$\left. - \delta j^*D^{-1}j - j^*D^{-1}\delta j\right) dx, \qquad (10b)$$

and integrating by parts gives

$$\delta J = \int_a^b \left\{ \delta\varphi^* \left[-\frac{d}{dx}\left(D\frac{d\varphi}{dx}\right) + \Lambda\varphi \right] + \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx} D\right) + \varphi^*\Lambda \right] \delta\varphi \right\} dx$$

$$+ \delta\varphi_-^* D_- \varphi_-' - \delta\varphi_+^* D_+ \varphi_+' + \varphi_-'^* D_- \delta\varphi_- - \varphi_+'^* \delta\varphi_+, \tag{10c}$$

and

$$\delta F = \int_a^b \left[\delta\varphi^* \left(\frac{dj}{dx} + \Lambda\varphi\right) - \delta j^* \left(\frac{d\varphi}{dx} + D^{-1} j\right) \right.$$

$$\left. + \left(\frac{dj^*}{dx} + \varphi^*\Lambda\right) \delta\varphi - \left(\frac{d\varphi^*}{dx} + j^* D^{-1}\right) \delta j \right] dx$$

$$+ \varphi_-^* \delta j_- - \varphi_+^* \delta j_+ - j_-^* \delta\varphi_- + j_+^* \delta\varphi_+. \tag{10d}$$

Since $\delta\varphi_-^*$, $\delta\varphi_+^*$, $\delta\varphi_-$, $\delta\varphi_+$, δj_-, and δj_+ are independent arbitrary variations, $\delta J = 0$ and $\delta F = 0$ imply the following conditions at x_0:

$$\varphi_-' = \varphi_+' = \varphi_-^{*\prime} = \varphi_+^{*\prime} = 0 \quad \text{for } J, \tag{11}$$

and

$$\varphi_-^* = \varphi_+^* = j_-^* = j_+^* = 0 \quad \text{for } F. \tag{12}$$

On physical grounds, the desired conditions at x_0 are

$$\left.\begin{aligned} \varphi_+ &= \varphi_-, & \varphi_+^* &= \varphi_-^* \\ D_+\varphi_+' &= D_-\varphi_-', & D_+\varphi_+^{*\prime} &= D_-\varphi_-^{*\prime} \end{aligned}\right\} \text{for } J, \tag{13}$$

and

$$\left.\begin{aligned} \varphi_+ &= \varphi_-, & \varphi_+^* &= \varphi_-^* \\ j_+ &= j_-, & j_+^* &= j_-^* \end{aligned}\right\} \text{for } F. \tag{14}$$

Clearly, the functionals $J[\varphi,\varphi^*]$ and $F[\varphi,\varphi^* j,j^*]$ will be stationary for functions φ, φ^* j, and j^* that do not satisfy the appropriate interface conditions at $x = x_0$ and are therefore unacceptable.

To obtain the proper interface condition, we must modify the functionals J and F, by adding terms defined at the interface.

The following modified functionals have their stationary value for functions φ, φ^*, j, and j^* which satisfy conditions 13 or 14 at $x = x_0$:

$$J_1[\varphi,\varphi^*] = (\varphi^*_+ - \varphi^*_-)\,\alpha + \beta(\varphi_+ - \varphi_-) + \int_a^b \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^*\Lambda\varphi\right) dx, \tag{15}$$

$$J_2[\varphi,\varphi^*] = \alpha(D_+\varphi'_+ - D_-\varphi'_-) + \beta(\varphi_+ - \varphi_-) + \int_a^b \varphi^*\left[\frac{d}{dx}\left(D\frac{d\varphi}{dx}\right) - \Lambda\varphi\right] dx, \tag{16}$$

$$J_3[\varphi,\varphi^*] = (\varphi^*_+ - \varphi^*_-)\,\alpha + (\varphi^{*\prime}_+ D_+ - \varphi^{*\prime}_- D_-)\,\beta + \int_a^b \left[\frac{d}{dx}\left(\frac{d\varphi^*}{dx} D\right) - \varphi^*\Lambda\right] \varphi\, dx, \tag{17}$$

$$J_4[\varphi,\varphi^*,\gamma] = (\varphi^*_+ - \varphi^*_-)[\gamma D_+\varphi'_+ + (1-\gamma)\, D_-\varphi'_-] + [\gamma\varphi^{*\prime}_+ D_+ + (1-\gamma)\,\varphi^{*\prime}_- D_-](\varphi_+ - \varphi_-)$$
$$+ \int_a^b \left(\frac{d\varphi^*}{dx} D \frac{d\varphi}{dx} + \varphi^*\Lambda\varphi\right) dx, \tag{18}$$

$$F_1[\varphi,\varphi^*,j,j^*] = \alpha(\varphi_+ - \varphi_-) + \beta(j_+ - j_-) + \int_a^b \left(\varphi^*\frac{dj}{dx} - j^*\frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \tag{19}$$

$$F_2[\varphi,\varphi^*,j,j^*] = \alpha(\varphi_+ - \varphi_-) + (\varphi^*_+ - \varphi^*_-)\,\beta$$
$$+ \int_a^b \left(-\frac{d\varphi^*}{dx} j - j^*\frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \tag{20}$$

$$F_3[\varphi,\varphi^*,j,j^*] = (j^*_+ - j^*_-)\,\alpha + \beta(j_+ - j_-)$$
$$+ \int_a^b \left(\varphi^*\frac{dj}{dx} + \frac{dj^*}{dx}\varphi + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \tag{21}$$

$$F_4[\varphi,\varphi^*,j,j^*] = (j^*_+ - j^*_-)\,\alpha + (\varphi^*_+ - \varphi^*_-)\,\beta$$
$$+ \int_a^b \left(\frac{dj^*}{dx}\varphi - \frac{d\varphi^*}{dx} j + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \tag{22}$$

and

$$F_5[\varphi,\varphi^*,j,j^*,\gamma] = [\gamma\varphi_-^* + (1-\gamma)\,\varphi_+^*](j_+ - j_-) - [\gamma j_+^* + (1-\gamma)\,j_-^*](\varphi_+ - \varphi_-)$$

$$+\int_a^b \left(\varphi^* \frac{dj}{dx} - j^* \frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \qquad (23)$$

where α and β are undetermined multipliers defined at the interface, and γ is a numerical parameter. Buslik[6] first proposed functionals $J_1[\varphi,\varphi^*]$ and $F_2[\varphi,\varphi^*,j,j^*]$. The functionals J_2, J_3, F_1, F_3, and F_4 are of the same type. Functional $J_4[\varphi,\varphi^*,\gamma]$ is of the type proposed by Pomraning[3] for the self-adjoint Sturm-Liouville equation. F_5 for $\gamma = 1/2$ coincides with the functional used by Wachspress and Becker,[2] and a similar form was proposed by Pomraning[3] for time-dependent problems.

We will now show that the stationarity conditions for $J_1[\varphi,\varphi^*]$, $J_4[\varphi,\varphi^*,\gamma]$, $F_1[\varphi,\varphi^*,j,j^*]$, and $F_5[\varphi,\varphi^*,j,j^*;\gamma]$ are the appropriate ones for the physical problem. The demonstration for J_2, J_3, F_2, F_3, and F_4 would essentially be the same and will thus not be carried out. The first variations for J_1, J_4, F_1, and F_5 are

$$\delta J_1 = \int_a^b \left\{\delta\varphi^*\left[-\frac{d}{dx}\left(D\frac{d\varphi}{dx}\right) + \Lambda\varphi\right] + \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}D\right) + \varphi^*\Lambda\right]\delta\varphi\right\} dx$$

$$+ (\varphi_+^* - \varphi_-^*)\,\delta\alpha + \delta\beta(\varphi_+ - \varphi_-) + \delta\varphi_-^*(D_-\varphi_-' - \alpha) + \delta\varphi_+^*(\alpha - D_+\varphi_+')$$

$$+ (\varphi_-^{*\prime}D_- - \beta)\,\delta\varphi_- + (\beta - \varphi_+^{*\prime}D_+)\,\delta\varphi_+, \qquad (24)$$

$$\delta J_4(\gamma) = \int_a^b \left\{\delta\varphi^*\left[-\frac{d}{dx}\left(D\frac{d\varphi}{dx}\right) + \Lambda\varphi\right] + \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}D\right) + \varphi^*\Lambda\right]\delta\varphi\right\} dx$$

$$+ (\varphi_+^* - \varphi_-^*)[\gamma D_+\delta\varphi_+' + (1-\gamma)\,D_-\delta\varphi_-'] + [\gamma\delta\varphi_+^{*\prime}D_+ + (1-\gamma)\,\delta\varphi_-^{*\prime}D_-](\varphi_+ - \varphi_-)$$

$$- [\gamma\delta\varphi_-^* + (1-\gamma)\,\delta\varphi_+^*](D_+\varphi_+' - D_-\varphi_-') - (\varphi_+^{*\prime}D_+ - \varphi_+^{*\prime}D_+)[\gamma\delta\varphi_- + (1-\gamma)\,\delta\varphi_+], \qquad (25)$$

$$\delta F_1 = \int_a^b \left[\delta\varphi^*\left(\frac{dj}{dx} + \Lambda\varphi\right) + \left(\frac{dj^*}{dx} + \varphi^*\Lambda\right)\delta\varphi - \delta j^*\left(\frac{d\varphi}{dx} + D^{-1}j\right)\right.$$

$$\left. - \left(\frac{d\varphi^*}{dx} + j^*D^{-1}\right)\delta j\right] dx + \delta\alpha(\varphi_+ - \varphi_-) + \delta\beta(j_+ - j_-)$$

$$+ (j_+^* + \alpha)\,\delta\varphi_+ - (\alpha + j_-^*)\,\delta\varphi_- + (\beta - \varphi_+^*)\,\delta j_+ + (\varphi_-^* - \beta)\,\delta j_-, \qquad (26)$$

and

$$\delta F_5(\gamma) = \int_a^b \left[\delta\varphi^*\left(\frac{dj}{dx} + \Lambda\varphi\right) + \left(\frac{dj^*}{dx} + \varphi^*\Lambda\right)\delta\varphi - \delta j^*\left(\frac{d\varphi}{dx} + D^{-1}j\right) \right.$$

$$\left. - \left(\frac{d\varphi^*}{dx} + j^*D^{-1}\right)\delta j \right] dx + [\gamma\delta\varphi_-^* + (1-\gamma)\,\delta\varphi_+^*](j_+ - j_-)$$

$$- [\gamma\delta j_+^* + (1-\gamma)\,\delta j_-^*](\varphi_+ - \varphi_-) + (j_+^* - j_-^*)[\gamma\delta\varphi_- + (1-\gamma)\,\delta\varphi_+]$$

$$- (\varphi_+^* - \varphi_-^*)[\gamma\delta j_+ + (1-\gamma)\,\delta j_-]. \tag{27}$$

The stationarity conditions as usual follow from requiring $\delta J_1 = \delta J_4 = \delta F_1 = \delta F_5 = 0$. In these cases, in the reactor volume, they are

$$\left.\begin{aligned} &-\frac{d}{dx}\left(D\,\frac{d\varphi}{dx}\right) + \Lambda\varphi = 0 \\ &\text{and} \\ &-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}\,D\right) + \varphi^*\Lambda = 0 \end{aligned}\right\} \text{ for } J_1 \text{ and } J_4; \tag{28}$$

$$\left.\begin{aligned} &\frac{dj}{dx} + \Lambda\varphi = 0, \\ &\frac{d\varphi}{dx} + D^{-1}j = 0, \\ &\frac{dj^*}{dx} + \varphi^*\Lambda = 0, \\ &\text{and} \\ &\frac{d\varphi^*}{dx} + j^*D^{-1} = 0 \end{aligned}\right\} \text{ for } F_1 \text{ and } F_5; \tag{29}$$

plus the following interface conditions:

$$\left.\begin{aligned} &\varphi_+ = \varphi_-, \\ &\varphi_+^* = \varphi_-^*, \\ &D_+\varphi_+' = D_-\varphi_-' = \alpha, \\ &\text{and} \\ &\varphi_+^{*\prime}D_+ = \varphi_-^{*\prime}D_- = \beta \end{aligned}\right\} \text{ for } J_1. \tag{30}$$

$$\left.\begin{aligned} \varphi_+ &= \varphi_-, \\ \varphi_+^* &= \varphi_-^*, \\ D_+\varphi_+' &= D_-\varphi_-', \\ \text{and} \quad & \\ \varphi_+^{*\prime} D_+ &= \varphi_-^{*\prime} D_- \end{aligned}\right\} \text{for } J_4; \tag{31}$$

$$\left.\begin{aligned} \varphi_+ &= \varphi_-, \\ j_+ &= j_-, \\ j_+^* &= j_-^* = -\alpha, \\ \text{and} \quad & \\ \varphi_+^* &= \varphi_-^* = \beta \end{aligned}\right\} \text{for } F_1, \tag{32}$$

and

$$\left.\begin{aligned} \varphi_+ &= \varphi_1, \\ j_+ &= j_-, \\ j_+^* &= j_-^*, \\ \text{and} \quad & \\ \varphi_+^* &= \varphi_-^* \end{aligned}\right\} \text{for } F_5. \tag{33}$$

These are the required differential equations and interface conditions. Consequently, any of the functionals J_1, J_4, F_1, or F_5 can be used for the formulation of a variational flux-synthesis approximation using discontinuous trial functions. The same conclusion applies to J_2, J_3, F_2, F_3, and F_4.

Just as it was shown before for J and F, the functionals J_1, J_2, J_3, J_4, F_1, F_2, F_3, F_4, and F_5 can be written in several equivalent forms.

For brevity, the different equivalent forms will be shown only for J_1, J_4, F_1, and F_5.

$$\begin{aligned} J_1 &= \varphi_-^*(D_-\varphi_-' - \beta) + \varphi_+^*(\beta - D_+\varphi_+') + \alpha(\varphi_+ - \varphi_-) + \int_a^b \left\{ \varphi^* \left[-\frac{d}{dx}\left(D\,\frac{d\varphi}{dx}\right) + \Lambda\varphi \right] \right\} dx \\ &= (\varphi_-^{*\prime} D_- - \alpha)\,\varphi_- + (\alpha - \varphi_+^{*\prime} D_+)\,\varphi_+ + (\varphi_+ - \varphi_-^*)\,\beta + \int_a^b \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}\,D\right) + \varphi^*\Lambda \right] \varphi\, dx; \end{aligned} \tag{34}$$

$$J_4(\gamma) = [\gamma\varphi_+^{*\prime}D_+ + (1-\gamma)\,\varphi_-^{*\prime}D_-](\varphi_+ - \varphi_-) - [\gamma\varphi_-^* + (1-\gamma)\,\varphi_+^*](D_+\varphi_+' - D_-\varphi_-')$$

$$+ \int_a^b \varphi^*\left[-\frac{d}{dx}\left(D\,\frac{d\varphi}{dx}\right) + \Lambda\varphi\right] dx$$

$$= (\varphi_+^* - \varphi_-^*)[\gamma D_+\varphi_+' + (1-\gamma)\,D_-\varphi_-'] - (\varphi_+^{*\prime}D_+ - \varphi_-^{*\prime}D_-)[\gamma\varphi_- + (1-\gamma)\,\varphi_+]$$

$$+ \int_a^b \left[-\frac{d}{dx}\left(\frac{d\varphi^*}{dx}\,D\right) + \varphi^*\Lambda\right]\varphi\,dx; \qquad (35)$$

$$F_1 = (\beta - \varphi_+^*)\,j_+ + (\varphi_-^* - \beta)\,j_- + \alpha(\varphi_+ - \varphi_-)$$

$$+ \int_a^b \left(-\frac{d\varphi^*}{dx}\,j - j^*\,\frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx$$

$$= (j_+^* + \alpha)\,\varphi_+ - (j_-^* + \alpha)\,\varphi_- + \beta(j_+ - j_-)$$

$$+ \int_a^b \left(\varphi^*\,\frac{dj}{dx} + \varphi\,\frac{dj^*}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx$$

$$= (j^* + \alpha)\,\varphi_+ - (j_-^* + \alpha)\,\varphi_- + (\beta - \varphi_+^*)\,j_+ + (\varphi_-^* - \beta)\,j_-$$

$$+ \int_a^b \left(\frac{dj^*}{dx}\,\varphi - \frac{d\varphi^*}{dx}\,j + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx, \qquad (36)$$

$$F_5(\gamma) = -[\gamma j_+^* + (1-\gamma)\,j_-^*](\varphi_+ - \varphi_-) - (\varphi_+^* - \varphi_-^*)[\gamma j_+ + (1-\gamma)\,j_-]$$

$$+ \int_a^b \left(-\frac{d\varphi^*}{dx}\,j - j^*\,\frac{d\varphi}{dx} + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx$$

$$= (j_+^* - j_-^*)[\gamma\varphi_- + (1-\gamma)\,\varphi_+] + [\gamma\varphi_-^* + (1-\gamma)\,\varphi_+^*](j_+ - j_-)$$

$$+ \int_a^b \left(\varphi^*\,\frac{dj}{dx} + \frac{dj^*}{dx}\,\varphi + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx$$

$$= (j_+^* - j_-^*)[\gamma\varphi_- + (1-\gamma)\,\varphi_+] - (\varphi_+^* - \varphi_-^*)[\gamma j_+ + (1-\gamma)\,j_-]$$

$$+ \int_a^b \left(\frac{dj^*}{dx}\,\varphi - \frac{d\varphi^*}{dx}\,j + \varphi^*\Lambda\varphi - j^*D^{-1}j\right) dx. \qquad (37)$$

SOME MATHEMATICAL PROBLEMS AND COMPARISON TO PREVIOUS WORK

In the preceding section, it was stated that integrals of sectionally continuous functions over [a,b] are well defined and finite. This statement is based on a fundamental theorem of the theory of integration. (See p. 163 of Ref. 7.) But since it seems to contradict Ref. 2 (p. 194), where it is argued that such integrals diverge, it is perhaps worthwhile to consider the problem in some detail.

Let $f_1(x)$ and $f_2(x)$ be two sectionally continuous functions, with sectionally continuous first derivatives, having jump discontinuities at $x = x_0$, where x_0 is assumed to be inside [a,b]. In Ref. 2, it is argued that under these conditions, the integral

$$\int_a^b f_1'(x)f_2'(x)\,dx,$$

where $f'(x) \equiv df(x)/dx$, diverges. This is based on the following argument:

The sectionally continuous function f(x), with a jump discontinuity at x_0, is approximated (for $|x - x_0| < \eta$, where $\eta > 0$) by

$$f(x) = \frac{f(x_0+\eta) + f(x_0-\eta)}{2} + \frac{x - x_0}{2\eta}\left[f(x_0+\eta) - f(x_0-\eta)\right]. \tag{38}$$

Let the right side of Eq. 38 be denoted by $f_\eta(x)$, in order to explicitly exhibit its dependence on the parameter η. The integral over [a,b] is then broken up in three integrals over the intervals $[a, x_0 - \eta]$, $[x_0 - \eta, x_0 + \eta]$ and $[x_0 + \eta, b]$. If one uses Eq. 38 to express $f_1(x)$ and $f_2(x)$ in the interval $|x - x_0| \le \eta$, and then calculates

$$\lim_{\eta\to+0} \int_{x_0-\eta}^{x_0+\eta} \frac{df_{1\eta}(x)}{dx}\frac{df_{2\eta}(x)}{dx}\,dx, \tag{39}$$

one finds that this indeed diverges. Thus one seems to be forced to conclude that

$$\int_a^b \frac{df_1(x)}{dx}\frac{df_2(x)}{dx}\,dx \tag{40}$$

diverges. That this conclusion is erroneous, however, can be easily demonstrated by considering the trivial case

$$f_1(x) = f_2(x) = \theta(x), \tag{41}$$

where $\theta(x)$ is the step function defined by

$$\left.\begin{aligned} \theta(x) &= 1 \quad \text{for } x > 0 \\ &= 0 \quad \text{for } x < 0. \end{aligned}\right\} \tag{42}$$

The derivative $d\theta/dx$ exists and is well defined and equal to zero for all x, except $x = 0$, which is a set of measure zero. It is obvious therefore that

$$\int_{-1}^{+1} \frac{d\theta}{dx}\frac{d\theta}{dx}\, dx = 0 \tag{43}$$

and not infinite, as Eq. 39 seems to imply.

The explanation of the discrepancy lies in the fact that, in general,

$$\int_a^b f_1' f_2'\, dx \neq \lim_{\eta\to+0}\left(\int_a^{x_0-\eta} f_{1\eta}' f_{2\eta}'\, dx + \int_{x_0-\eta}^{x_0+\eta} f_{1\eta}' f_{2\eta}'\, dx + \int_{x_0+\eta}^{b} f_{1\eta}' f_{2\eta}'\, dx\right). \tag{44}$$

What one actually does in approximating the discontinuous function f(x), as in Eq. 38, is express f(x) as the limit of a sequence of functions $f_\eta(x)$ for $\eta \to +0$. The sequence $\{f_\eta(x)\}$ does indeed converge to f(x) as $\eta \to +0$, but the convergence is not uniform. That this convergence is not uniform can be readily seen using the usual (ϵ, δ) reasoning. But without going into that proof, all one has to observe is that the functions $f_\eta(x)$ are continuous in the interval $[x_0 - \eta, x_0 + \eta]$, while f(x) is discontinuous at x_0 which is contained in the above interval for all η. And, according to a basic theorem of Real Analysis (p. 239 of Ref. 7), if a sequence of continuous functions converges uniformly to some function, then that limit function must be continuous. Therefore, $f_\eta(x)$ cannot converge uniformly to f(x). Since this convergence is not uniform, all one can say is that

$$\int_a^b \left[\lim_{\eta\to+0}\left(f_{1\eta}' f_{2\eta}'\right)\right] dx = \int_a^b f_1'(x) f_2'(x)\, dx, \tag{45}$$

but the limit cannot generally be taken after the integration (see, for example, Ref. 7, p. 241). It is precisely for this reason that expressions 39 and 40 do not give the same result. Thus the divergence appearing in Ref. 2 is an artifact of the calculation and not a property of sectionally continuous functions.

Another apparent ambiguity that has appeared in the literature[3,8] is the assertion that, if one uses discontinuous functions in an integral of the form

$$\int_a^b f(x)g'(x)\, dx,$$

then one is led to ambiguous integrals of the form

$$\int_a^b \theta(x - x_0)\, \delta(x - x_0)\, dx,$$

where $\theta(x)$ is the step function and $\delta(x)$ the delta function. Evidently, the basis for this statement seems to lie in the assumption that if, for example, one has the integral

$$\int_a^b \theta(x - x_0)\, \theta'(x - x_0)\, dx, \tag{46}$$

where x_0 is inside [a,b], then one can replace $\theta'(x - x_0)$ by the delta function. Again, that this cannot be the case is easily seen if one recalls that $\theta'(x - x_0)$ is zero for all $x \neq x_0$, and therefore Eq. 46 vanishes; if one introduces the delta function, the resulting expression is meaningless (see also Eq. 56).

To resolve the difficulty, one should recall the conditions under which the derivative of a discontinuous function can be interpreted as a delta function. Let $\varphi(x)$ be a function that is bounded and continuous everywhere in a closed interval [a,b] and is also infinitely differentiable everywhere in [a,b]. Let f(x) be a function that has a jump discontinuity at x_0 (which is assumed to be inside [a,b]) and be continuous, differentiable, and bounded otherwise. Let it be assumed, for simplicity, that both functions vanish at $x = a$ and $x = b$. Consider now the integral

$$\int_a^b f(x)\varphi'(x)\, dx,$$

and break it up in two integrals over the intervals $[a, x_0 - \epsilon]$ and $[x_0 + \epsilon, b]$. Each of the two integrals can then be integrated by parts and the limit for $\epsilon \to +0$ be taken. The result is

$$\int_a^b f(x)\varphi'(x)\, dx = -\Delta f\varphi(x_0) - \int_a^b \varphi(x)f'(x)\, dx, \tag{47}$$

where

$$\Delta f = \lim_{\epsilon \to +0} f(x_0 + \epsilon) - \lim_{\epsilon \to +0} f(x_0 - \epsilon) = f^+ - f^- . \tag{48}$$

Now, since $\varphi(x)$ is continuous, differentiable, etc., in $[a,b]$, and in particular at x_0, one can write

$$\varphi(x_0) = \int_a^b \varphi(x)\delta(x - x_0)\, dx, \tag{49}$$

and, upon substituting Eq. 49 into Eq. 47, one obtains

$$\int_a^b f(x)\varphi'(x)\, dx = -\int_a^b [\Delta f \delta(x - x_0) + f'(x)\varphi(x)]\, dx. \tag{50}$$

Introducing the symbol $\tilde{f}'(x)$, defined by

$$\tilde{f}'(x) = f'(x) + \Delta f \delta(x - x_0), \tag{51}$$

one can write Eq. 50 in the form

$$\int_a^b f(x)\varphi'(x)\, dx = -\int_a^b \tilde{f}'(x)\varphi(x)\, dx. \tag{52}$$

The above derivation is contained in more detail in Ref. 9.

What Eqs. 51 and 52 imply is that, as far as integration by parts with a continuous function such as $\varphi(x)$ is concerned, the derivative of a discontinuous function can be interpreted as a generalized function (or distribution); and the tilde on $\tilde{f}'$ is intended to indicate explicitly that it is a generalized function. Of course, $f'(x)$ which appears in Eq. 51 is the usual derivative of the discontinuous function $f(x)$; it exists and is well defined for all $x \in [a,b]$, except for x_0. This interpretation of the derivative of a discontinuous function as a generalized function enables one to preserve Eq. 52, which otherwise is valid only for continuous functions. But only with test functions $\varphi(x)$ that are continuous, differentiable, etc.* is Eq. 51 valid.

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* The delta function can be used in an integral of the form

$$\int_{-\infty}^{+\infty} g(x)\delta(x)\, dx,$$

with $g(x)$ being continuous but not differentiable at $x = 0$. For example, $g(x)$ may have a "corner" at $x = 0$, in which case its derivative is discontinuous at $x = 0$. In that case, however, one loses the differentiability properties that such inner products have. This means that integrals of the form

$$\int_{-\infty}^{+\infty} g(x)\delta'(x)\, dx$$

(where $\delta'(x)$ is the derivative of the delta function) are then meaningless. When $g(x)$ is infinitely differentiable, such integrals are meaningful with derivatives of $\delta(x)$ of any order.[9] But when $g(x)$ itself is discontinuous at $x = 0$, the integral

$$\int_{-\infty}^{+\infty} g(x)\delta(x)\, dx$$

is meaningless.

Moreover, even in that case, Eq. 51 is meaningful only when used in the inner product* of Eq. 52 and cannot be given a pointwise interpretation. That is, if one has an integral of the form

$$\int \varphi(x) f'(x)\, dx,$$

where f(x) is discontinuous, one cannot simply replace $f'(x)$ by $\tilde{f}'(x)$. This is precisely what is implied in Ref. 3, p. 622, and it is for this reason that the meaningless integral arises. That the pointwise interpretation of Eq. 51 is wrong was illustrated with Eq. 46, which led to a meaningless integral. The following example shows that it also leads to contradictions.

Consider the integral

$$\int_{-\infty}^{+\infty} \theta'(x - x_0)\, dx.$$

Clearly, this is zero because $\theta'(x - x_0) = 0$ for all x except x_0. If, however, one uses Eq. 51 for the derivative, one finds $\tilde{\theta}'(x - x_0) = \delta(x - x_0)$ and

$$\int_{-\infty}^{+\infty} \delta(x - x_0)\, dx = 1,$$

which is a contradiction.

Having established that the identification of the derivatives of discontinuous functions with delta functions is meaningful only in the context of integration by parts with infinitely differentiable test functions, one is tempted to ask whether discontinuous test functions might be included. For the answer, one has to go back to Eq. 47. If $\varphi(x)$ also had a jump discontinuity at x_0, Eq. 47 would read

$$\int_a^b f(x)\varphi'(x)\, dx = -(f^+\varphi^+ - f^-\varphi^-) - \int_a^b \varphi(x) f'(x)\, dx, \tag{53}$$

and this is as far as one can go. Thus, Eq. 51 is not applicable in this case. Instead, one has to work with Eq. 53 without delta functions, and this is what was done in the second section of this report.

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*Strictly speaking, the defining equation of the derivative of a discontinuous function[10] f(x) is Eq. 52, which is often written as $\langle \tilde{f}'(x), \phi(x)\rangle = -\langle f(x), \phi'(x)\rangle$. Then, Eq. 51 is just a way of computing $\tilde{f}'(x)$ that the above equation defines. Similarly the second derivative is defined by $\langle \tilde{f}''(x), \phi(x)\rangle = \langle f(x), \phi''(x)\rangle$, and so on.

For some purposes, one can assign an arbitrary value to a discontinuous function at the point of discontinuity. For example, in the theory of Fourier series, it is natural and convenient to assign the value $\frac{1}{2}(f^+ + f^-)$. One must be aware, however, that this freedom does not exist in Eq. 47. If one attempts to apply Eq. 47 for the case in which both f(x) and $\varphi(x)$ are discontinuous at x_0, by assigning to $\varphi(x_0)$ say the value $\frac{1}{2}(\varphi^+ + \varphi^-)$, a contradiction will result. This can be shown by integrating the right side of Eq. 47 by parts once more. The resulting contradiction is

$$(\varphi^+ - \varphi^-)(f^+ + f^-) = (\varphi^+ + \varphi^-)(f^+ - f^-). \tag{54}$$

This equation obviously is not valid for arbitrary discontinuous functions f(x) and $\varphi(x)$.

It has been suggested in Ref. 3 (p. 631), and a calculation presumably supporting the suggestion has been given, that one can "demand" that the integral

$$\beta = \int_{-\infty}^{+\infty} \theta(x)\delta(x)\, dx$$

be meaningful and furthermore that integration by parts be valid. The associated calculation leads to the value 1/2. In that calculation, integration by parts is performed by using $\tilde{\theta}'(x) = \delta(x)$. This leads to the relation

$$\int_{-\infty}^{+\infty} \theta(x)\delta(x)\, dx = 1 - \int_{-\infty}^{+\infty} \theta(x)\theta'(x)\, dx. \tag{55}$$

Replacing then $\theta'(x)$ by $\delta(x)$, one is led to the value $\beta = 1/2$.

But one could also observe that the integral

$$\int_{-\infty}^{+\infty} \theta(x)\theta'(x)\, dx,$$

in the right-hand side of Eq. 55 is well defined and equal to zero. Then Eq. 55 would give $\beta = 1$. Moreover, if the pointwise interpretation of the relation $\tilde{\theta}'(x) = \delta(x)$ were valid, one could write

$$\beta = \int_{-\infty}^{+\infty} \theta(x)\delta(x)\, dx = \int_{-\infty}^{+\infty} \theta(x)\theta'(x)\, dx = 0. \tag{56}$$

The last two values, 1 and 0 for β, contradict the value 1/2 found in Ref. 3 and subsequently used in Ref. 8.

Thus the same manipulations lead to different values for β depending on the sequence of the manipulations. First of all, integration by parts of the integral

$$\int_{-\infty}^{+\infty} \theta(x)\delta(x)\, dx,$$

as performed in Ref. 3, would not be allowed even if $\delta(x)$ were replaced by a continuous function, because in that case one would lose surface terms arising from the discontinuity of $\theta(x)$ at $x = 0$ (see Eq. 47). Of course, the presence of the delta function, complicates matters even more, and integration by parts simply is not permitted. But the crux of the matter is that no meaning can be given to the integral

$$\int_{-\infty}^{+\infty} \theta(x)\delta(x)\, dx.$$

In connection with this problem, the reader is also referred to an erudite analysis from a somewhat different viewpoint by Bremermann and Durand.[11]

The conclusion therefore is that sectionally continuous functions can be used in functionals of the type given in Eqs. 1 and 2, without giving rise to divergences. Moreover, the meaningless (or ambiguous) integrals that have appeared in the literature are due to improper use of the delta function. As has been shown, the introduction of delta functions is neither appropriate nor necessary.

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